10/666811

STRUCTURE FILE UPDATES: 15 SEP 2005 HIGHEST RN 863287-86-9
DICTIONARY FILE UPDATES: 15 SEP 2005 HIGHEST RN 863287-86-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

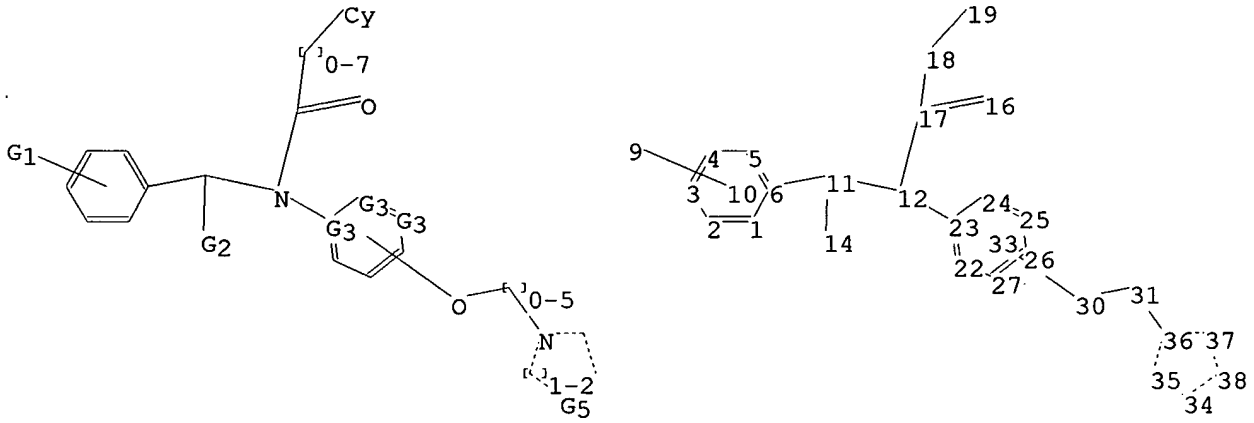
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10666811\10666811j.str



chain nodes :
9 11 12 14 16 17 18 19 30 31
ring nodes :
1 2 3 4 5 6 22 23 24 25 26 27 34 35 36 37 38
chain bonds :
6-11 11-12 11-14 12-17 12-23 16-17 17-18 18-19 30-31 31-36
ring bonds :

```
1-2  1-6  2-3  3-4  4-5  5-6  22-23  22-27  23-24  24-25  25-26  26-27  34-35
34-38  35-36  36-37  37-38
exact/norm bonds :
6-11  11-12  11-14  12-17  12-23  16-17  17-18  18-19  22-23  22-27  23-24  24-25
25-26  26-27  30-31  31-36  34-35  34-38  35-36  36-37  37-38
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6


G1:H,OH,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,CN,X,Ak

G2:Ak,H

G3:C,N

G4:H,Cy,Ak

G5:O,S,C

Hydrogen count :
11:>= minimum 1
Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  9:CLASS  10:CLASS  11:CLASS
12:CLASS  14:CLASS  16:CLASS  17:CLASS  18:CLASS  19:Atom  22:Atom  23:Atom
24:Atom  25:Atom  26:Atom  27:Atom  30:CLASS  31:CLASS  33:CLASS  34:Atom  35:Atom
36:Atom  37:Atom  38:Atom



L1      STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s L1
SAMPLE SEARCH INITIATED 15:16:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      331 TO ITERATE

100.0% PROCESSED      331 ITERATIONS                                  1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          5529 TO     7711
PROJECTED ANSWERS:                1 TO       80

L2            1 SEA SSS SAM L1

=> s L1 full
FULL SEARCH INITIATED 15:16:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     6833 TO ITERATE

100.0% PROCESSED     6833 ITERATIONS                                 60 ANSWERS
SEARCH TIME: 00.00.01

L3           60 SEA SSS FUL L1
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=> fil caplus
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 161.33 | 161.75

FILE 'CAPLUS' ENTERED AT 15:16:30 ON 16 SEP 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 16 Sep 2005 VOL 143 ISS 13
FILE LAST UPDATED: 15 Sep 2005 (20050915/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

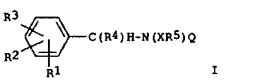
=> s L3
L4 2 L3

=> d ibib abs 1-2

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:267292 CAPLUS
DOCUMENT NUMBER: 140:287259
TITLE: Preparation of amide and sulfonamide ligands for the estrogen receptor
INVENTOR(S): O'Keefe Cameron, Kimberly; Chesworth, Richard
PATENT ASSIGNEE(S): Pfizer Products Inc., USA
SOURCE: PCT Int. Appl., 143 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004026823	A1	20040401	WO 2003-IB3824	20030908
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2499490	AA	20040401	CA 2003-2499490	20030908
EP 1542967	A1	20050622	EP 2003-797427	20030908
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003014126	A	20050628	BR 2003-14126	20030908
US 2004110767	A1	20040610	US 2003-666811	20030917
PRIORITY APPLN. INFO.:			US 2002-412338P	P 20020920
			WO 2003-IB3824	W 20030908

OTHER SOURCE(S): MARPAT 140:287259
GI



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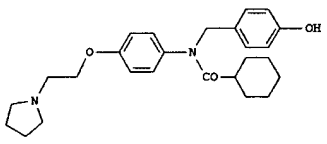


II

AB The present invention provides amides and sulfonamides (shown as I; variables defined below; many of the examples contain the pyrrolidine ring, e.g. II) that are estrogen receptor (ER) ligands (no data), the pharmaceutically acceptable salts, stereoisomers, and prodrugs thereof,

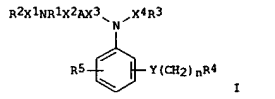
L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
and the pharmaceutically acceptable salts of the prodrugs. The invention further provides pharmaceutical compns. comprising I, and methods for treating or preventing diseases, disorders, conditions, or symptoms mediated by an ER (e.g. female sexual dysfunction, postmenopausal syndrome, osteoporosis, elevated serum cholesterol levels, and breast or uterine cancer) which comprise administering to a mammalian subject in need of treatment therewith, an effective amt. of I, or a pharmaceutically acceptable salt, stereoisomer, or prodrug thereof, or a pharmaceutically acceptable salt of the prodrug, or a pharmaceutical compn. comprising I, or a pharmaceutically acceptable salt, stereoisomer, or prodrug thereof, or a pharmaceutically acceptable salt of the prodrug. The invention further provides pharmaceutical compns. comprising combinations of I and ≥1 of NaF, estrogen, a bone anabolic agent, a growth hormone or growth hormone secretagogue, a prostaglandin agonist/antagonist, and a parathyroid hormone, and methods of treating or preventing diseases, disorders, conditions, or symptoms mediated by an ER comprising the administration of an effective amt. of such combination to a mammalian subject in need of treatment therewith. Although the methods of prepn. are not claimed, 212 example prepns. are included. For example, II was prepd. in 41% yield by base hydrolysis of its p-toluenesulfonic acid ester, which in turn was prepd. N-acylation of toluene-4-sulfonic acid 4-[[[4-[2-(pyrrolidin-1-yl)ethoxy]phenyl]amino]methyl]phenyl ester by cyclohexanecarbonyl chloride. Toluene-4-sulfonic acid 4-[[[4-[2-(pyrrolidin-1-yl)ethoxy]phenyl]amino]methyl]phenyl ester was prepd. in 2 steps (71 and 80%, resp., yields) starting with tosylate formation from 4-hydroxybenzaldehyde followed by imine formation with [4-[2-(pyrrolidin-1-yl)ethoxy]phenyl]amine and redn. by NaBH4. For I: Q = R9- and Z-substituted Ph or six-membered heteroaryl ring contg. 1-2 N atoms; R1, R2, R3, and R9 are H, hydroxy, halogen, cyano, -(C1-C6) alkyl (un)substituted with 1-3 F atoms and -O(C1-C6)alkyl (un)substituted with 1-3 F atoms. R4 is H or -(C1-C6)alkyl; R5 is -(C1-C7)alkyl (un)substituted with 1-6 halogen atoms, -(C2-C6) alkenyl, -(C2-C6)alkenyl-M, or -(CH2)n-M, wherein n = 0-5 and M is (i) a fully satd. 3-8 membered ring, or a partially satd., or fully satd. 5-8 membered ring optionally having = 1-4 heteroatoms independently O, N, and S, or (ii) a bicyclic ring comprising two fused partially satd., fully satd., or fully unsatd. 5- or 6-membered rings optionally having 1-4 heteroatoms independently O, N and S. X is CO or SO2; Z is -O(CH2)n-NRaRb, -(CH2)n-NRaRb, -CH:CH-C(O)-NRaRb, -(CH2)n-COOH, -CH:CH-COOH, -O(C1-C6)alkyl, -CH:CH-CO2(C1-C6)alkyl, or -(CH2)n-OH; addnl. details are given in the claims.
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:833284 CAPLUS
DOCUMENT NUMBER: 135:371641
TITLE: Preparation of arylheterocyclylamides as motilin antagonists
INVENTOR(S): Johnson, Sigmond G.; Rivero, Ralph A.
PATENT ASSIGNEE(S): Ortho-McNeil Pharmaceutical, Inc., USA
SOURCE: PCT Int. Appl., 132 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001085694	A2	20011115	WO 2001-US11821	20010411
WO 2001085694	A3	20020404		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002013352	A1	20020131	US 2001-829767	20010410
US 6511980	B2	20030128		
CA 2408288	AA	20011115	CA 2001-2408288	20010411
EP 1294695	A2	20030326	EP 2001-926866	20010411
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003532710	T2	20031105	JP 2001-582295	20010411
BG 107243	A	20030731	BG 2002-107243	20021101
US 2003203906	A1	20031030	US 2002-291133	20021108
US 2005148584	A1	20050707	US 2005-66202	20050225
PRIORITY APPLN. INFO.:			US 2000-202131P	P 20000505
			US 2001-829767	A3 20010410
			WO 2001-US11821	W 20010411
			US 2002-291133	A3 20021108

OTHER SOURCE(S): MARPAT 135:371641
GI

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)



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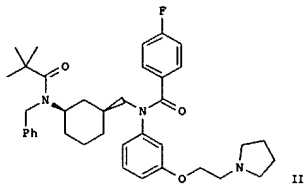

II

AB Title compds. [I; R1 = H, (substituted) aryl, aralkyl, heterocyclyl, diarylalkyl, alkyl, etc.; R2 = (substituted) aryl, aralkyl, cycloalkyl, heterocyclyl, heterocyclylalkyl, etc.; X1-X4 = null, CO, SO2; R1NR2X1 = (substituted) heterocyclyl; A = (substituted) alkyl, alkenyl, cycloalkyl, cycloalkylalkyl, etc.; Y = O, NH, S, SO2; n = 0-5; R4 = H, amino, alkylamino, dialkylamino, heterocyclyl, alkylheterocyclyl, etc.], were prepared Thus, N-[3-[2-(1-pyrrolidino)ethoxy]phenyl]-N-(cis-3-aminocyclohexyl)methyl-4-fluorophenylcarboxamide (preparation given) and PhCHO in PhMe were treated sequentially with Ti(OiPr)4, EtOH, and NaBH(OAc)3 to give a crude residue which in CH2Cl2 was treated with Me3CCOCl to give title compound (II). II inhibited motilin-induced contraction in rabbit colon with IC50 = 0.029 μM.

has close structure but does not read on amended at R5 & R1

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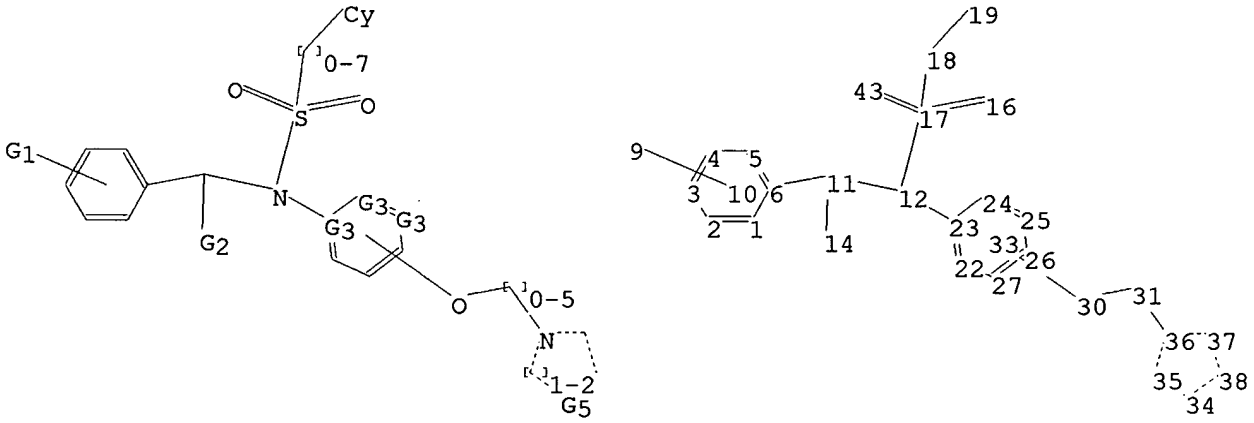
* available and contains the CA role and document type information. *
*
****

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10666811\10666811i.str



chain nodes :
9 11 12 14 16 17 18 19 30 31 43
ring nodes :
1 2 3 4 5 6 22 23 24 25 26 27 34 35 36 37 38
chain bonds :
6-11 11-12 11-14 12-17 12-23 16-17 17-18 17-43 18-19 30-31 31-36
ring bonds :

```
1-2  1-6  2-3  3-4  4-5  5-6  22-23  22-27  23-24  24-25  25-26  26-27  34-35
34-38  35-36  36-37  37-38
exact/norm bonds :
6-11  11-12  11-14  12-17  12-23  16-17  17-18  17-43  18-19  22-23  22-27  23-24
24-25  25-26  26-27  30-31  31-36  34-35  34-38  35-36  36-37  37-38
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6


G1:H,OH,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,CN,X,Ak

G2:Ak,H

G3:C,N

G4:H,Cy,Ak

G5:O,S,C

Hydrogen count :
11:>= minimum 1
Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  9:CLASS  10:CLASS  11:CLASS
12:CLASS  14:CLASS  16:CLASS  17:CLASS  18:CLASS  19:Atom  22:Atom  23:Atom
24:Atom  25:Atom  26:Atom  27:Atom  30:CLASS  31:CLASS  33:CLASS  34:Atom  35:Atom
36:Atom  37:Atom  38:Atom  43:CLASS



L1      STRUCTURE UPLOADED

=> s L1
SAMPLE SEARCH INITIATED 15:12:15 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       71 TO ITERATE

100.0% PROCESSED       71 ITERATIONS                                  11 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          915 TO     1925
PROJECTED ANSWERS:              22 TO      418

L2           11 SEA SSS SAM L1

=> s L1 full
FULL SEARCH INITIATED 15:12:22 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     1380 TO ITERATE

100.0% PROCESSED     1380 ITERATIONS                                191 ANSWERS
SEARCH TIME: 00.00.02

L3          191 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     161.33     161.75

FILE 'CAPLUS' ENTERED AT 15:12:27 ON 16 SEP 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 16 Sep 2005 VOL 143 ISS 13
FILE LAST UPDATED: 15 Sep 2005 (20050915/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L3
L4 1 L3

=> d ibib abs

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:267292 CAPLUS
DOCUMENT NUMBER: 140:287259
TITLE: Preparation of amide and sulfonamide ligands for the estrogen receptor
INVENTOR(S): O'Keefe Cameron, Kimberly; Chesworth, Richard
PATENT ASSIGNEE(S): Pfizer Products Inc., USA
SOURCE: PCT Int. Appl., 143 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004026823	A1	20040401	WO 2003-IB3824	20030908
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
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EP 1542967	A1	20050622	EP 2003-797427	20030908
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US 2004110767	A1	20040610	US 2003-666811	20030917
PRIORITY APPLN. INFO.:			US 2002-412338P P	20020920
			WO 2003-IB3824 W	20030908

OTHER SOURCE(S): MARPAT 140:287259
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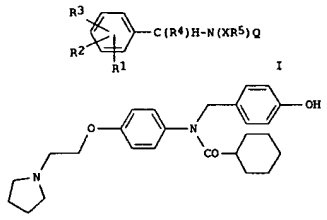

I

II

AB The present invention provides amides and sulfonamides (shown as I; variables defined below; many of the examples contain the pyrrolidine ring, e.g. II) that are estrogen receptor (ER) ligands (no data), the pharmaceutically acceptable salts, stereoisomers, and prodrugs thereof, and the pharmaceutically acceptable salts of the prodrugs. The invention further provides pharmaceutical compns. comprising I, and methods for treating or preventing diseases, disorders, conditions, or symptoms mediated by an ER (e.g. female sexual dysfunction, postmenopausal syndrome, osteoporosis, elevated serum cholesterol levels, and breast or uterine cancer) which comprise administering to a mammalian subject in need of treatment therewith, an effective amt. of I, or a pharmaceutically acceptable salt, stereoisomer, or prodrug thereof, or a pharmaceutically acceptable salt of the prodrug, or a pharmaceutical compn. comprising I, or a pharmaceutically acceptable salt, stereoisomer, or prodrug thereof, or a pharmaceutically acceptable salt of the prodrug. The invention further provides pharmaceutical compns. comprising combinations of I and ≥1 of NaF, estrogen, a bone anabolic agent, a growth hormone or growth hormone secretagogue, a prostaglandin agonist/antagonist, and a parathyroid hormone, and methods of treating or preventing diseases, disorders, conditions, or symptoms mediated by an ER comprising the administration of an effective amt. of such combination to a mammalian subject in need of treatment therewith. Although the methods of prepn. are not claimed, 212 example prepns. are included. For example, II was prepd. in 41% yield by base hydrolysis of its p-toluenesulfonic acid ester, which in turn was prepd. N-acylation of toluene-4-sulfonic acid 4-{[[4-{2-(pyrrolidin-1-yl)ethoxy]phenyl]amino]methyl]phenyl ester by cyclohexanecarbonyl chloride. Toluene-4-sulfonic acid 4-[[[4-{2-(pyrrolidin-1-yl)ethoxy]phenyl]amino]methyl]phenyl ester was prepd. in 2 steps (71 and 80%, resp., yields) starting with tosylate formation from 4-hydroxybenzaldehyde followed by imine formation with [4-[2-(pyrrolidin-1-yl)ethoxy]phenyl]amine and redn. by NaBH4. For I: Q = R9- and Z-substituted Ph or six-membered heteroaryl ring contg. 1-2 N atoms; R1, R2, R3, and R9 are H, hydroxy, halogen, cyano, -(C1-C6) alkyl (un)substituted with 1-3 F atoms and -O(C1-C6)alkyl (un)substituted with 1-3 F atoms. R4 is H or -(C1-C6)alkyl; R5 is -(C1-C7)alkyl (un)substituted with 1-6 halogen atoms, -(C2-C6) alkenyl, -(C2-C6)alkenyl-M, or -(CH2)n-M, wherein n = 0-5 and M is (i) a fully satd. 3-8 membered ring, or a partially satd., or fully satd. 5-8 membered ring optionally having = 1-4 heteroatoms independently O, N, and S, or (ii) a bicyclic ring comprising two fused partially satd., fully satd., or fully unsatd. 5- or 6-membered rings optionally having 1-4 heteroatoms independently O, N and S. X is CO or SO2; Z is -O(CH2)n-NRaRb, -(CH2)n-NRaRb, -CH:CH-C(O)-NRaRb, -(CH2)n-COOH, -CH:CH-COOH, -O(C1-C6)alkyl, -CH:CH-CO2(C1-C6)alkyl, or -(CH2)n-OH; addnl. details are given in the claims.

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT